Bayesian Analysis for Complex Physical Systems Modeled by Computer Simulators: Current Status and Future Challenges

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practical/methodological (how can we work out what climate is likely to be?)

and

foundational (why should our methods work and what do our answers mean?)

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Climate change Large scale climate simulators are constructed to assess likely effects of human intervention upon future climate behaviour.
Aims are both scientific - much is unknown about the large scale interactions which determine climate - and also very practical, as such simulators provide evidence for the importance of changing human behaviour before possibly irreversible changes are set into motion.

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(ix) decision uncertainty (to use the model to influence real world outcomes, we need to relate things in the world that we can influence to inputs to the simulator and through outputs to actual impacts. These links are uncertain.)

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[In a climate model, y_h might correspond to historical climate outcomes over space and time, y to current and future climate, and the "decisions" might correspond to different policy relevant choices such as carbon emission scenarios.]

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$$z = y_h \oplus e, \;\; y = f(x^*) \oplus \epsilon$$

where e, ϵ have some appropriate probabilistic specification, possibly involving parameters which require estimation.

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Current state of the art

Many people work on different aspects of these uncertainty analyses

Great resource: the Managing Uncertainty in Complex Models web-site

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and it is hard!

RAPID-WATCH

What are the implications of RAPID-WATCH observing system data and other recent observations for estimates of the risk due to rapid change in the MOC? In this context risk is taken to mean the probability of rapid change in the MOC and the consequent impact on climate (affecting temperatures, precipitation, sea level, for example). This project must:

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* investigate how observations of the MOC can be used to constrain estimates of the probability of rapid MOC change, including magnitude and rate of change;
* make sound statistical inferences about the real climate system from model simulations and observations;
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* assess model uncertainty in climate impacts and characterise impacts that have received less attention (eg frequency of extremes).

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So, it is not unreasonable that the objective of our analysis should be probabilities which are asserted by at least one person (more would be good!).

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- “optimise” the performance of the system

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Full Bayes analysis can be more informative if done extremely carefully, both in terms of the prior specification and the analysis. Bayes linear analysis is partial but easier, faster, more robust particularly for history matching and forecasting.

Bayes linear approach

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(i) it is difficult to give a meaningful full prior probability specification over high dimensional spaces;
(ii) the computations, for learning from data (observations and computer runs), particularly when choosing informative runs, may be technically difficult;
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However, the idea of the Bayesian approach, namely capturing our expert prior judgements in stochastic form and modifying them by appropriate rules given observations, is conceptually appropriate (and there is no obvious alternative).

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(ii) the computations, for learning from data (observations and computer runs), particularly when choosing informative runs, may be technically difficult;
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However, the idea of the Bayesian approach, namely capturing our expert prior judgements in stochastic form and modifying them by appropriate rules given observations, is conceptually appropriate (and there is no obvious alternative).
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For a full account, see
Michael Goldstein and David Wooff (2007) Bayes Linear Statistics: Theory and Methods, Wiley.

Bayes linear adjustment

Bayes Linear adjustment of the mean and the variance of y given z is

$$\mathsf{E}_z[y] = \mathrm{E}(y) + \mathrm{Cov}(y,z)\mathrm{Var}(z)^{-1}(z - \mathrm{E}(z)),$$
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The foundation for the approach is an explicit treatment of temporal uncertainty, and the underpinning mathematical structure is the inner product space (not probability space, which is just a special case).

Function emulation

Uncertainty analysis, for high dimensional problems, is even more challenging if the function $f(x)$ is expensive, in time and computational resources, to evaluate for any choice of x. [For example, large climate models.]

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We use the emulator either to provide a full joint probabilistic description of all of the function values (full Bayes) or to assess expectations variances and covariances for pairs of function values (Bayes linear).

Form of the emulator

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$$\mathrm{Corr}(u_i(x), u_i(x')) = \exp(-(\tfrac{\|x-x'\|}{\theta_i})^2)$$

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We need careful (multi-output) experimental design to choose informative model evaluations, and detailed diagnostics to check emulator validity.

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We use this form as the prior for the emulator for $f_i(x)$.

Then a relatively small number of evaluations of $f_i(x)$, using relations such as

$$\beta_{ij} = \alpha_i \beta_{ij}' + \gamma_{ij}$$

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[This approach exploits the heuristic that we need many more function evaluations to identify the qualitative form of the model (i.e. choose appropriate forms $g_{ij}(x)$, etc) than to assess the quantitative form of all of the terms in the model - particularly if we fit meaningful regression components.]

Illustration from RAPID (thanks to Danny Williamson)

One of the main aims of the RAPIT programme is to assess the risk of shutdown of the AMOC (Atlantic Meridionnal Overturning Circulation)which transports heat from the tropics to Northern Europe and how this risk depends on the future emissions scenario for $CO2$.

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We had access to some runs of FAMOUS (a lower resolution model), which consisted of 6 scenarios for future CO2 forcing, and between 40 and 80 runs of FAMOUS under each scenario, with different parameter choices.

[And very little time to do the analysis.]

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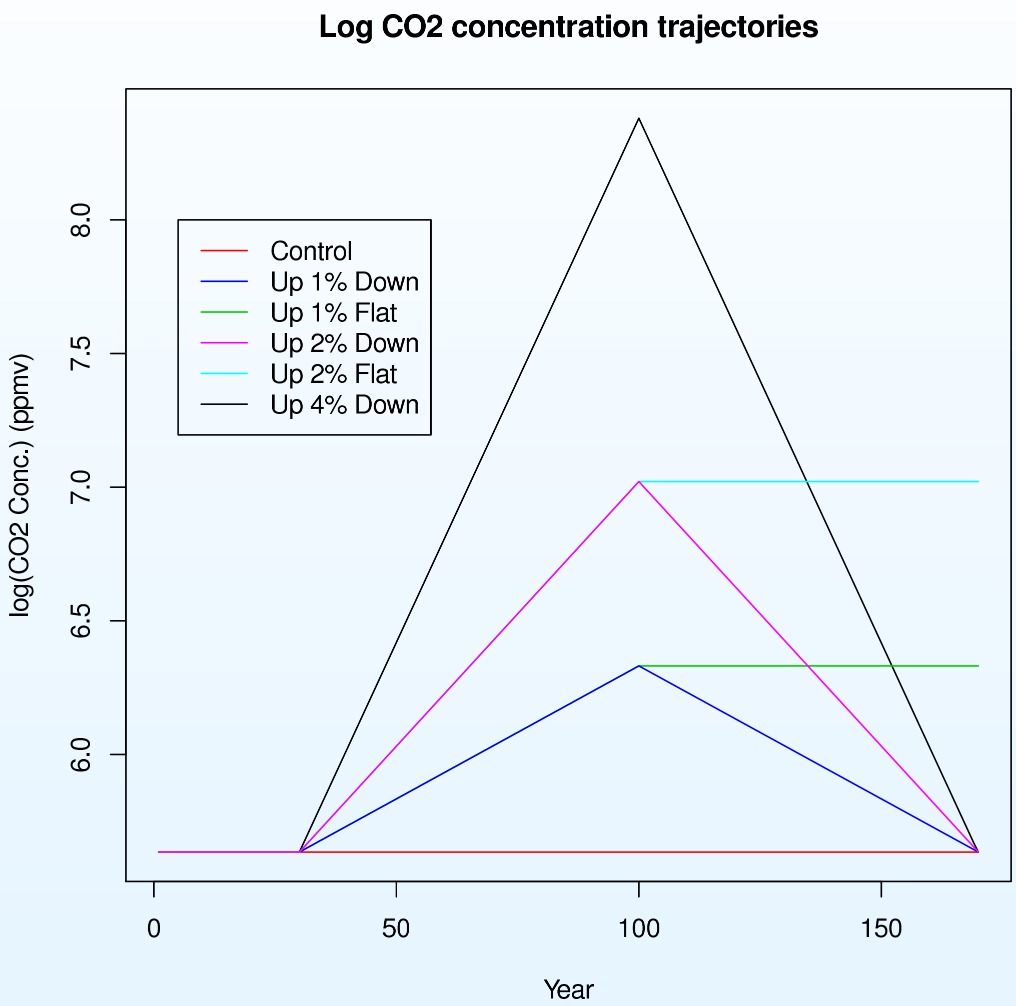
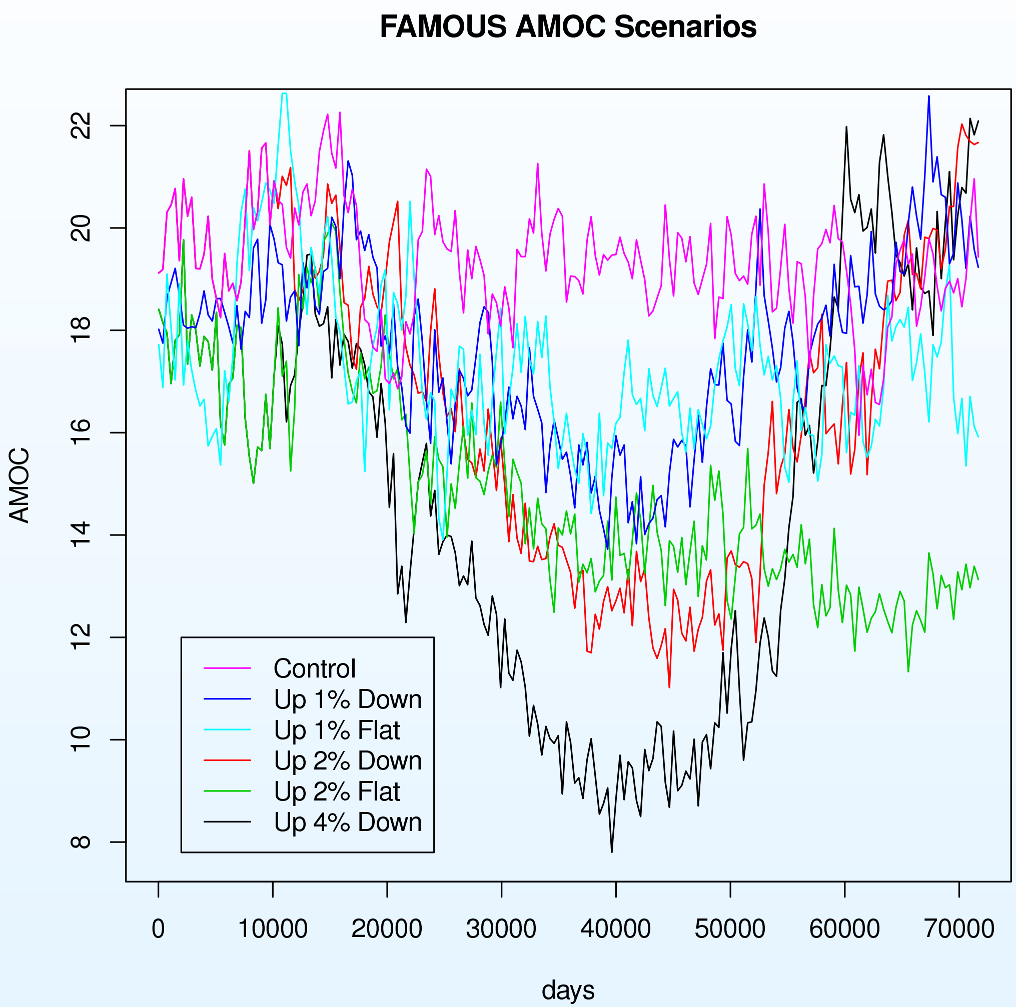
Our output of interest was a 170 year time series of AMOC values. The series is noisy and and the location and direction of spikes in the series was not important. Interest concerned aspects such as the value and location of the smoothed minimum of the series and the amount that AMOC responds to CO2 forcing and recovers if CO2 forcing is reduced.

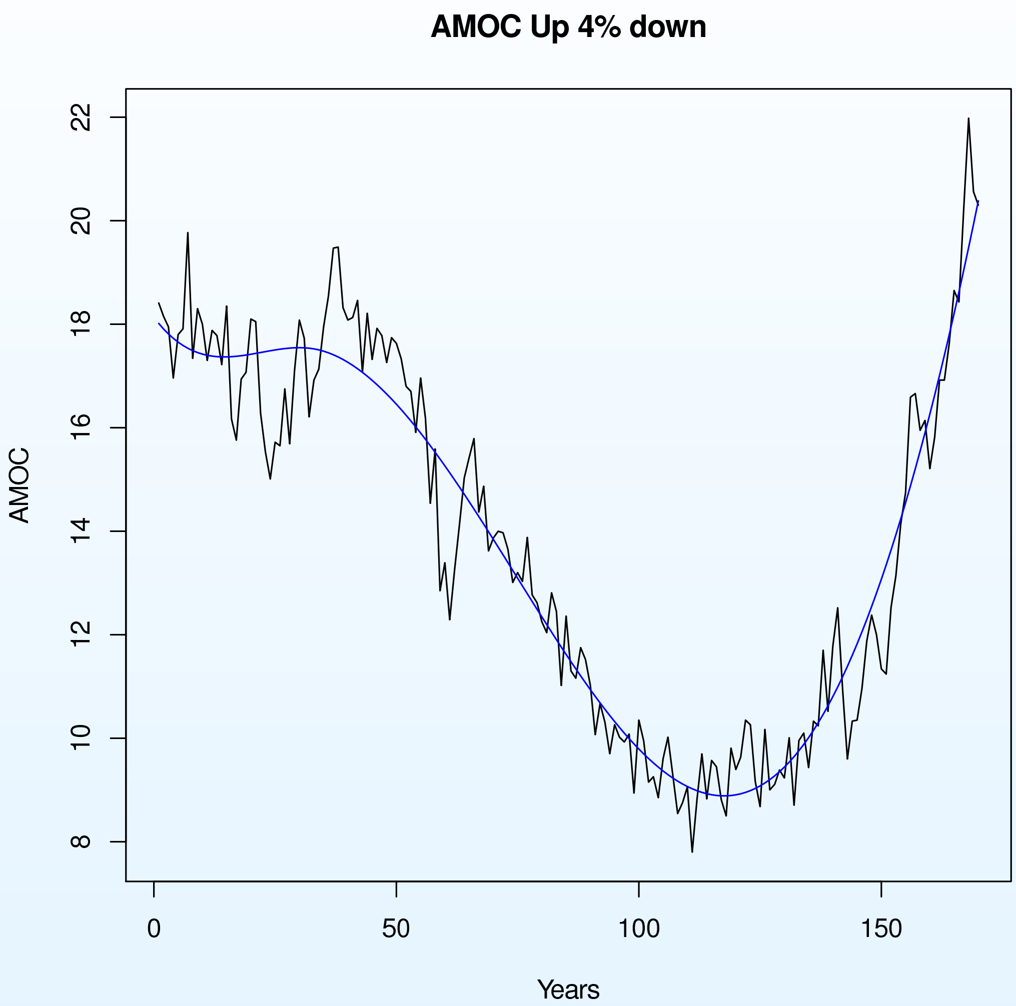
CO2 Scenarios



Famous Scenarios



Smoothing



We smooth by fitting splines $f^s(x,t) = \Sigma_j c_j(x) B_j(t)$ where $B_j(t)$ are basis functions over t and $c_j(x)$ are chosen to give the 'best' smooth fit to the time series.

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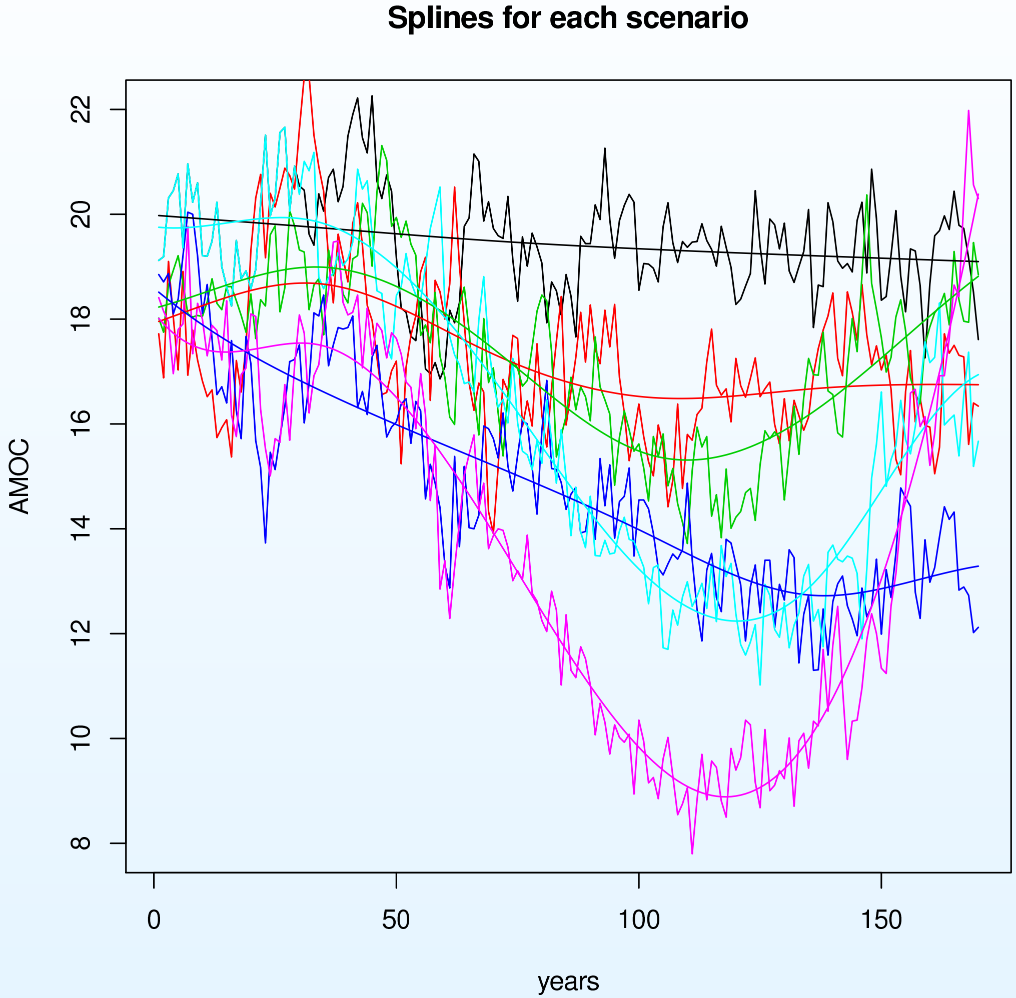
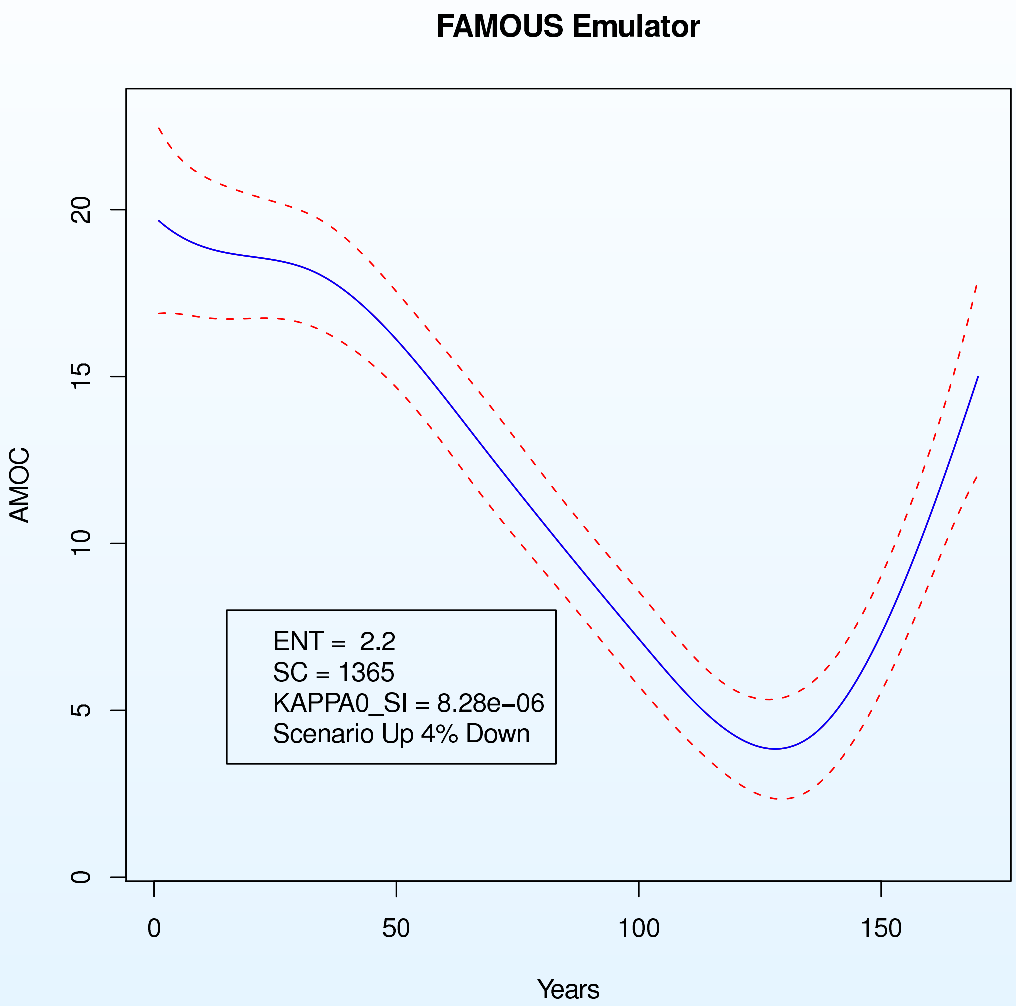


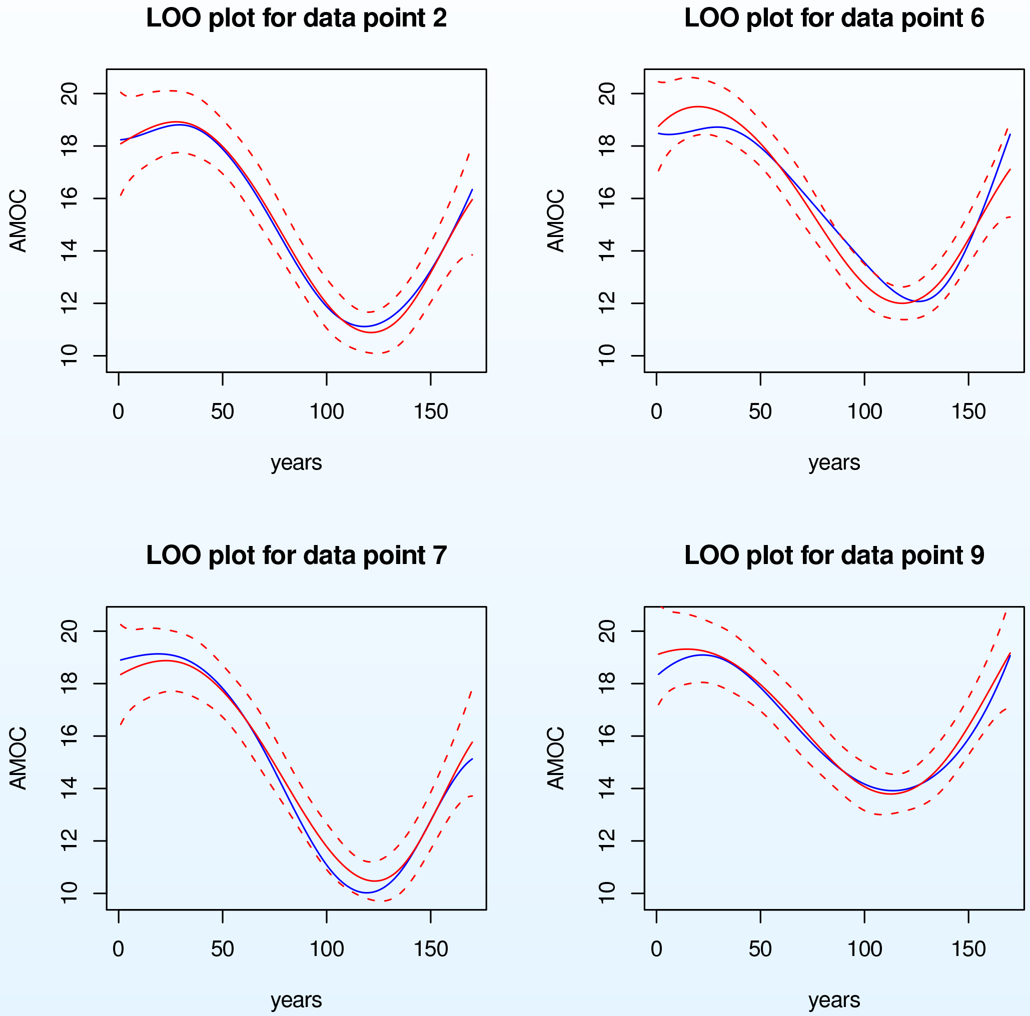
Splines for each scenario
AMOC
years
8
10
12
14
16
18
20
22
0
50
100
150

FAMOUS emulation



We emulate f^s by emulating each coefficient $c_j(x)$ in $f^s(x,t) = \Sigma_j c_j(x) B_j(t)$ (separately for each CO2 scenario)

Diagnostics (leave one out)



We test our approach by building emulators leaving out each observed run in turn, and checking whether the run falls within the stated uncertainty limits.

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[1] Extend the FAMOUS emulator across all choices of CO2 scenario.

[We do this using fast geometric arguments, exploiting the speed of working in inner product spaces. For example, we have a different covariance matrix for local variation at each of 6 CO2 scenarios. We extend this specification to all possible CO2 scenarios by identifying each covariance matrix as an element of an appropriate inner product space, and adjusting beliefs over covariance matrix space by projection.]

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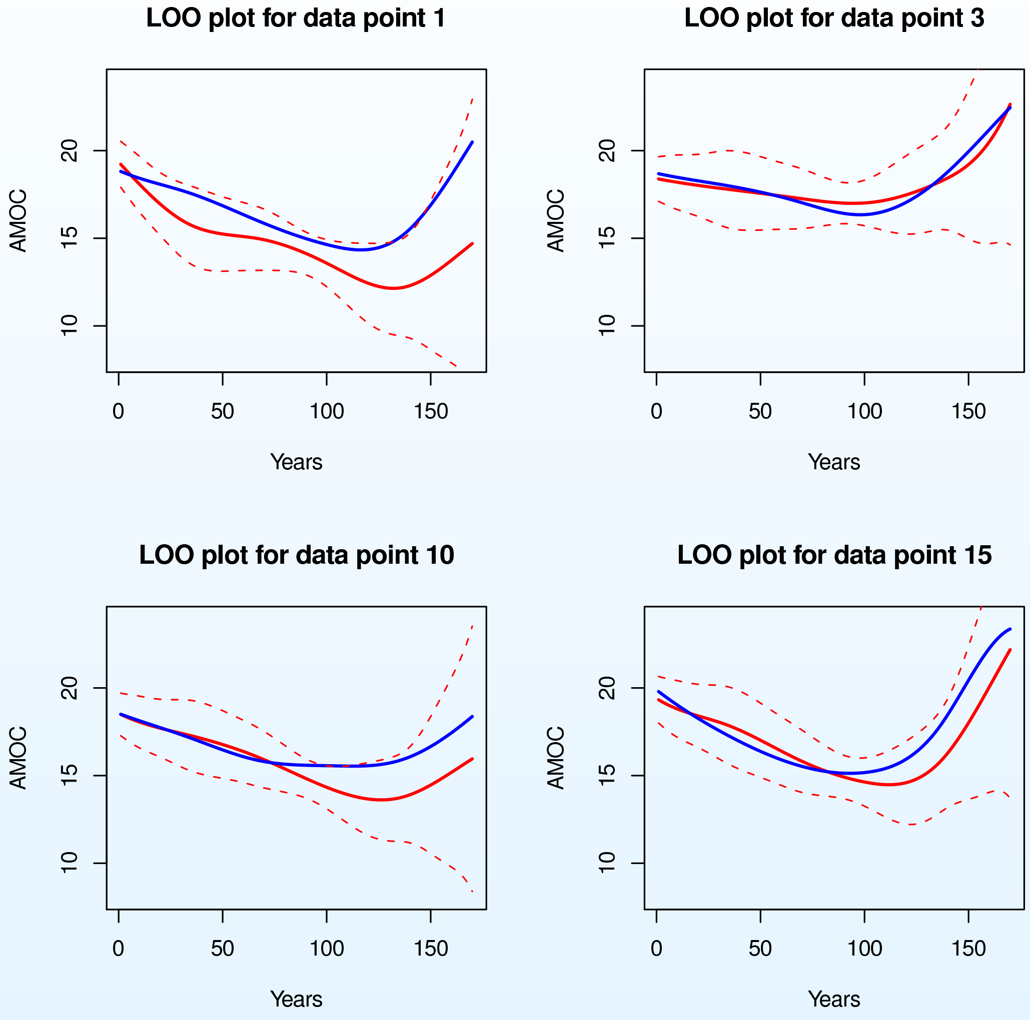
[4] Diagnostic checking, tuning etc.

Emulating HadCM3:diagnostics



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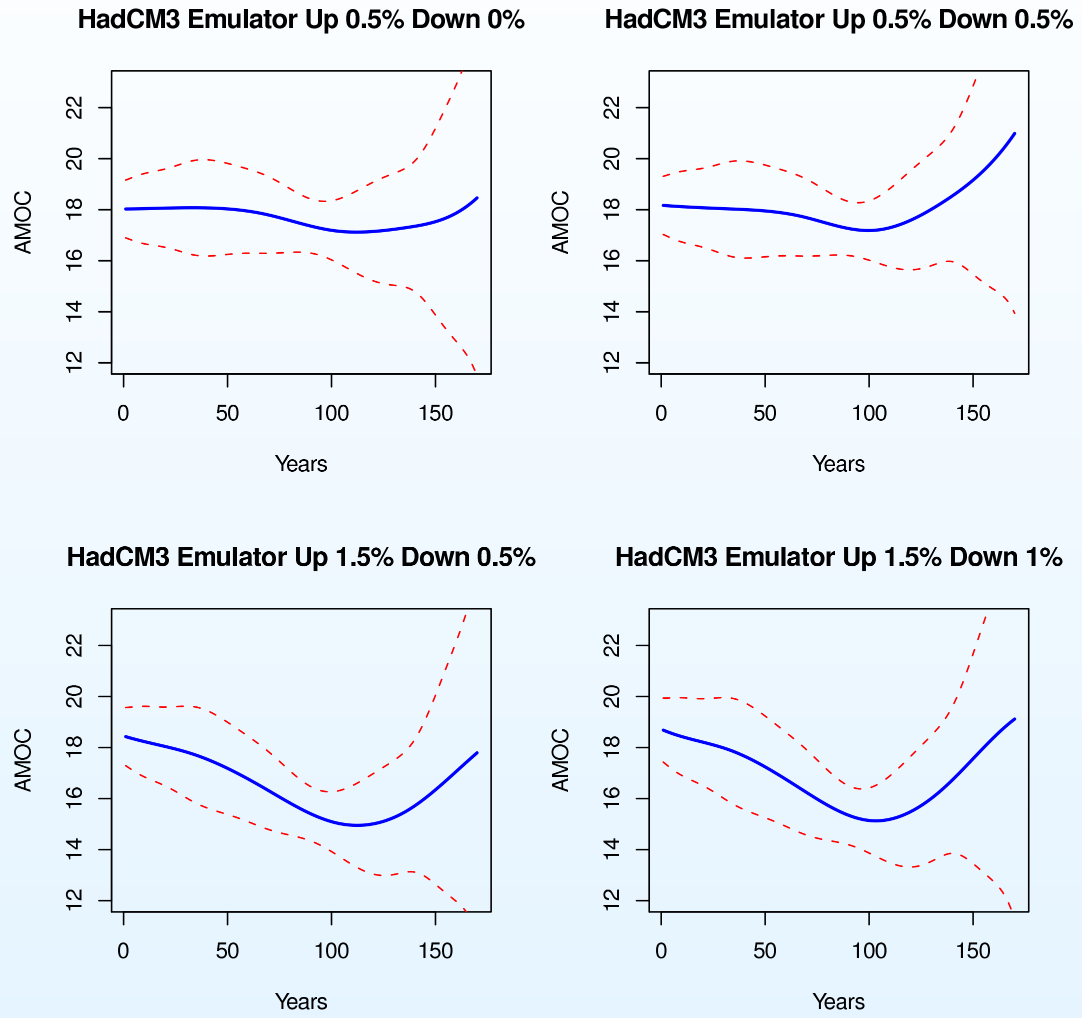

Example: Oil Reservoirs

- A oil reservoir is an underground region of porous rock which contains oil and/or gas. The hydrocarbons are trapped above by a layer of impermeable rock and below by a body of water, thus creating the reservoir. The oil and gas are pumped out of the reservoir and fluids are pumped into the reservoir (to boost production).

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- Example - Oil field containing 650 wells, 1 million plus grid cells (permeability, porosity, fault lines, etc.). Previous history match took one man-year of effort. Our methods found a match using 32 runs, each lasting 4 hours and automatically chosen with a overall fourfold improvement in fit.

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Outputs

- The model outputs comprise the behaviour of the various wells and injectors in the reservoir
- Output is a time series on the following variables for each well
    - *Pressures* Bottom-hole pressure, Tubing head pressure
    - *Production/Injection rates and totals* for each of oil, water and gas.
    - *Fluid ratios* Water cut, Gas-oil ratio
- The resolution of the time series can be varied from months to years
- With a large number of wells, daily output, or a long operating period there will be a *lot* of output data

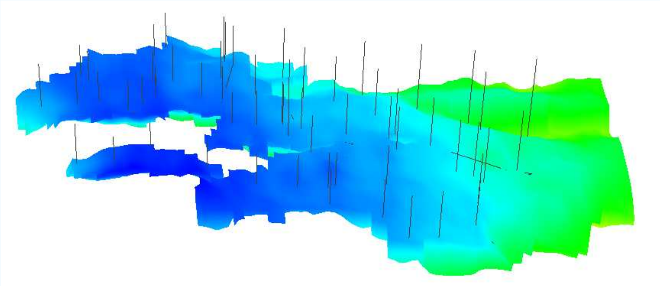
A reservoir example: (thanks to Jonathan Cumming)

Durham University

The model, based on grid size $38 \times 87 \times 25$, with 43 production and 13 injection wells, simulates 10 years of production, 1.5–3 hours per simulation.

Inputs Field multipliers for porosity (ϕ), permeabilities (k_x, k_z), critical saturation (crw), and aquifer properties (A_p, A_h)

Outputs Oil production rate for a 3-year period, for the 10 production wells active in that period. 4-month averages over the time series



Emulator for reservoir simulator is: $f_i(\boldsymbol{x}) = \boldsymbol{g}_i(\boldsymbol{x}_{[i]})\boldsymbol{\beta}_i + u_i(\boldsymbol{x}_{[i]}) + v_i(\boldsymbol{x})$

$\boldsymbol{g}_i(\boldsymbol{x}_{[i]})^T\boldsymbol{\beta}_i$ – a global trend function which captures the gross features, $\boldsymbol{x}_{[i]}$ – a subset of inputs which account for most of the variation in F, the *active variables*, $u_i(\boldsymbol{x}_{[i]})$ – a correlated residual process representing the local behaviour in the active variables, $v_i(\boldsymbol{x})$ – an uncorrelated 'nugget' residual.

Coarse and Accurate Emulators

The computer model is expensive to evaluate, so we use ‘coarse’ model, F^c,to capture qualitative features of F. F^c is substantially faster, allowing many model runs. We construct emulator f^c of F^c from these runs and a framework linking f^c and f. We make (small) number of runs of F, and update our emulator f.

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(linked via the equations relating the pairs of coefficients)

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(linked via the equations relating the pairs of coefficients)

Careful choice of small design to evaluate for full simulator allows us to (Bayes linear) update emulator for F based on prior emulator and additional runs.

Emulation Summaries

Well	Time	$\boldsymbol{x}_{[i]}$	No. Model Terms	Coarse Simulator R^2	Accurate Simulator $\tilde{R}^2$
B2	4	ϕ, crw, A_p	9	0.886	0.951
B2	8	ϕ, crw, A_p	7	0.959	0.958
B2	12	ϕ, crw, A_p	10	0.978	0.995
B2	16	ϕ, crw, k_z	7	0.970	0.995
B2	20	ϕ, crw, k_x	11	0.967	0.986
B2	24	ϕ, crw, k_x	10	0.970	0.970
B2	28	ϕ, crw, k_x	10	0.975	0.981
B2	32	ϕ, crw, k_x	11	0.980	0.951
B2	36	ϕ, crw, k_x	11	0.983	0.967

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In practice, we proceed by sequentially ruling out regions of x space which are unlikely to give rise to observed history z.

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We can therefore calculate, for each output $F_i(x)$, the "implausibility" if we consider the value x to be the best choice x^*, which is the standardised distance between z_i and $\mathrm{E}(F_i(x))$, which is

$$I_{(i)}(x) = |z_i - \mathrm{E}(F_i(x))|^2 / [\mathrm{Var}(F_i(x)) + \mathrm{Var}(\epsilon_i) + \mathrm{Var}(e_i)]$$

[Large values of $I_{(i)}(x)$ suggest that it is implausible that $x = x^*$.]

Using Implausibility measures

The implausibility calculation can be performed univariately, or by multivariate calculation over sub-vectors. The implausibilities are then combined, such as by using $I_M(x) = \max_i I_{(i)}(x)$, and can then be used to identify regions of x with large $I_M(x)$ as implausible, i.e. unlikely to be good choices for x^*.

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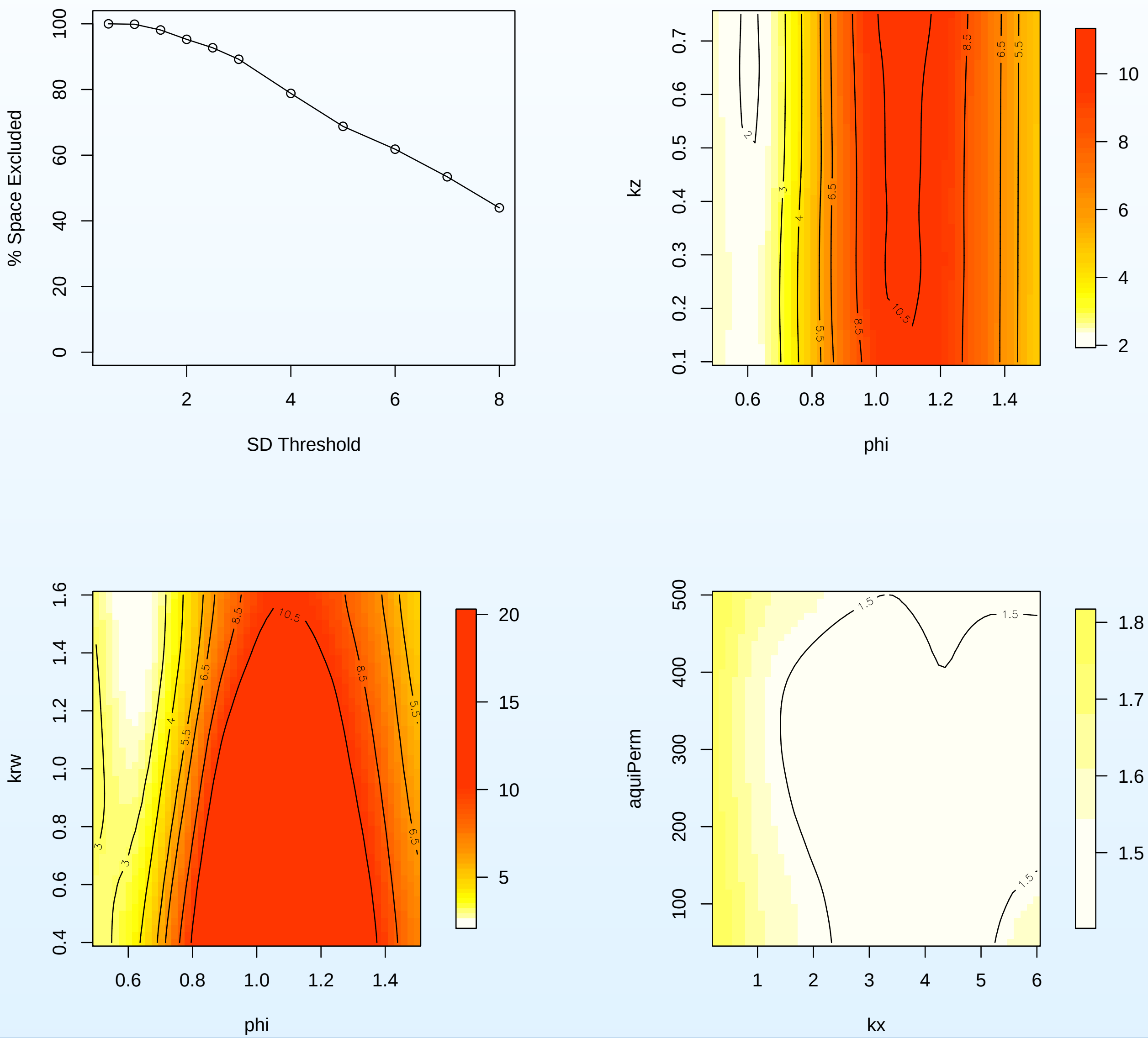
Comment: Even if calibrating, it is good practice to history match first, to check model and (massively) reduce search space.

Implausibility Results



Refocusing

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- Now consider final 4 time points in original data, plus an additional point 1 year beyond the end of the previous series to be forecast
- Since reducing the space many of the old model runs are no longer valid, so supplement with additional evaluations
- 262+100 coarse runs, 6+20 accurate runs
- Re-fit the coarse and fine emulators, using the old emulator structure as a starting point

Forecasting

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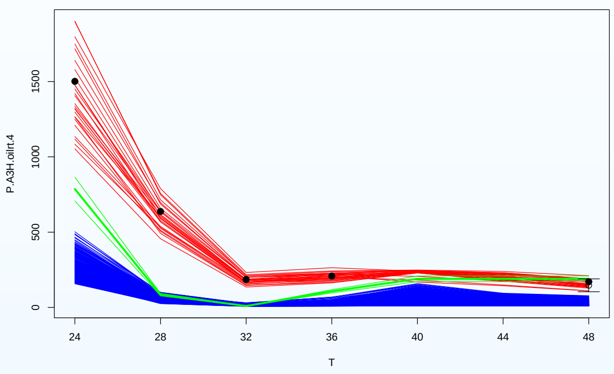
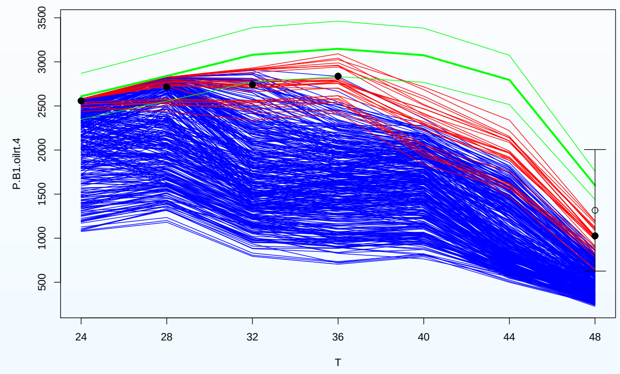
Comment Our computer experiments to forecast y_p split into two stages

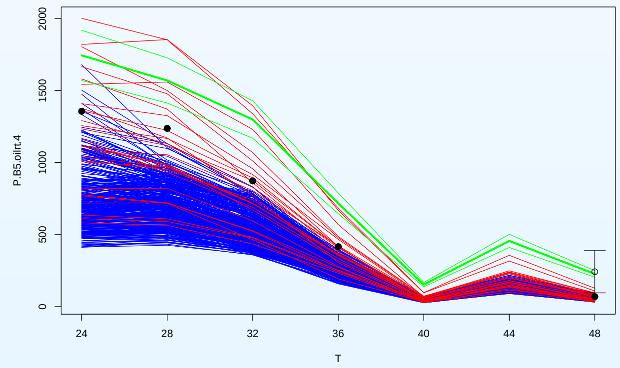
(i) preliminary simulator evaluations to identify the form of emulator, estimate coefficient matrices and refocus

(ii) further simulator evaluations chosen to minimise adjusted forecast variance.

Forecasting Results







Simulator outputs, observational data and forecasts for each well.

Green lines indicate z with error bounds of 2sd(e).

Red and blue lines represent the range of the runs of $F(x)$ and $F^c(x)$

Solid black dots correspond to $\mathrm{E}(F^*)$.

The forecast is indicated by a hollow circle with attached error bars.

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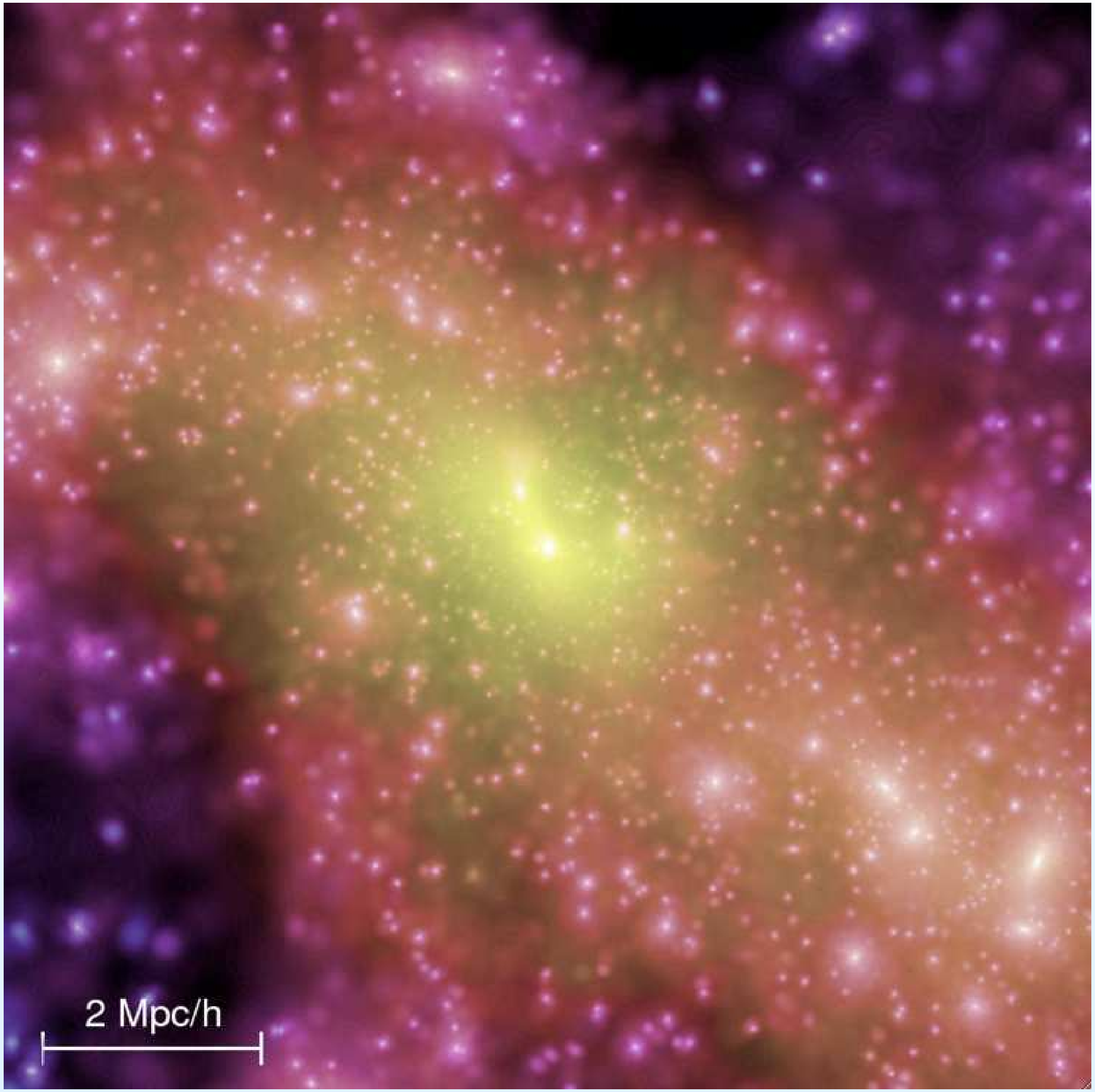
- The Galform model produces lots of outputs, some of which can be compared to observed data from the real Universe.

The Dark Matter Simulation

Durham University



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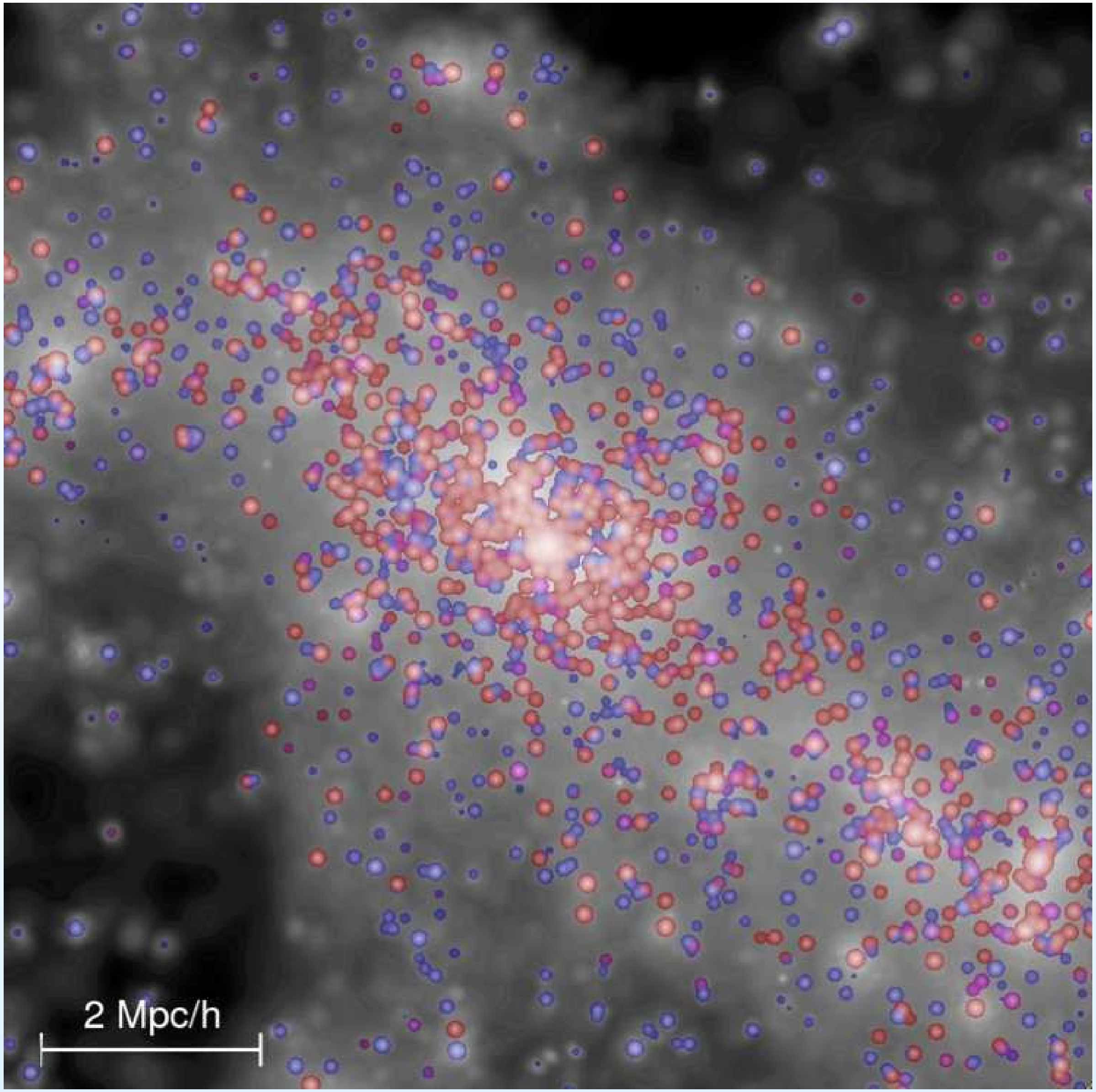

Inputs

To perform one run, we need to specify the following 17 inputs:

vhotdisk:	100 - 550	**VCUT**:	20 - 50
aReheat:	0.2 - 1.2	**ZCUT**:	6 - 9
alphacool:	0.2 - 1.2	**alphastar**:	-3.2 - -0.3
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We choose 11 outputs that are representative of the Luminosity functions and emulate the functions $f_i(x)$.

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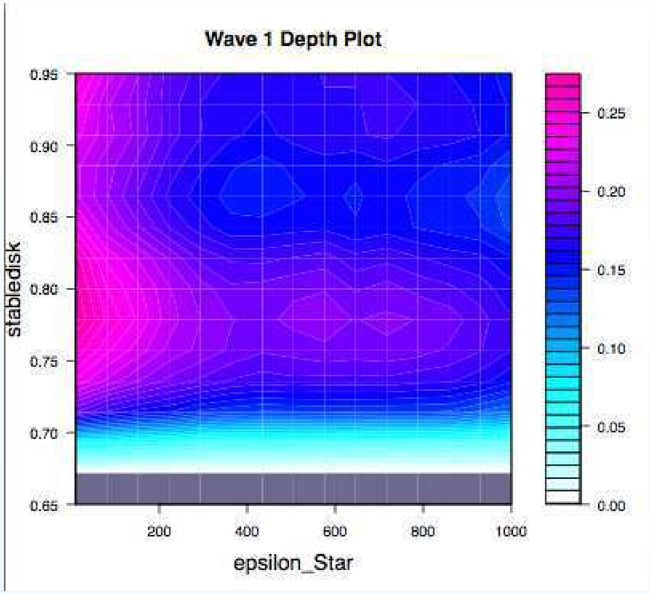
	No. Model Runs	No. Active Vars	Space Remaining
Wave 1	1000	5	14.9 %
Wave 2	1414	8	5.9 %
Wave 3	1620	8	1.6 %
Wave 4	2011	10	0.12 %

2D Implausibility Projections: Wave 1 (14%) to Wave 4 (0.12%)



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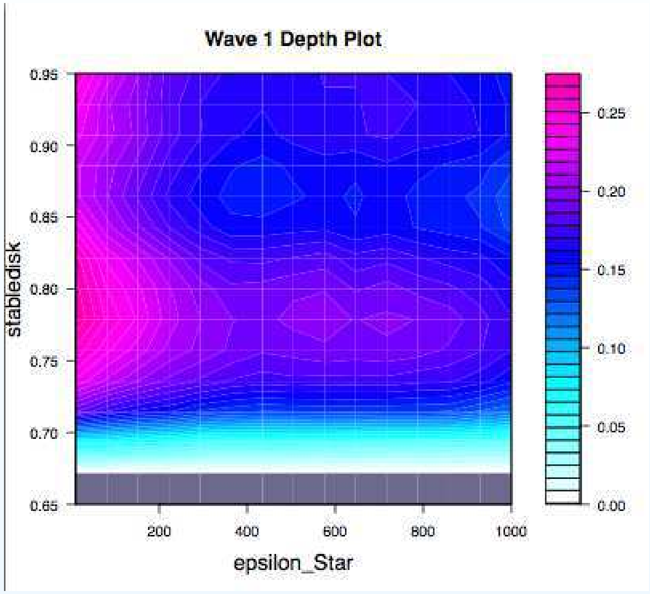

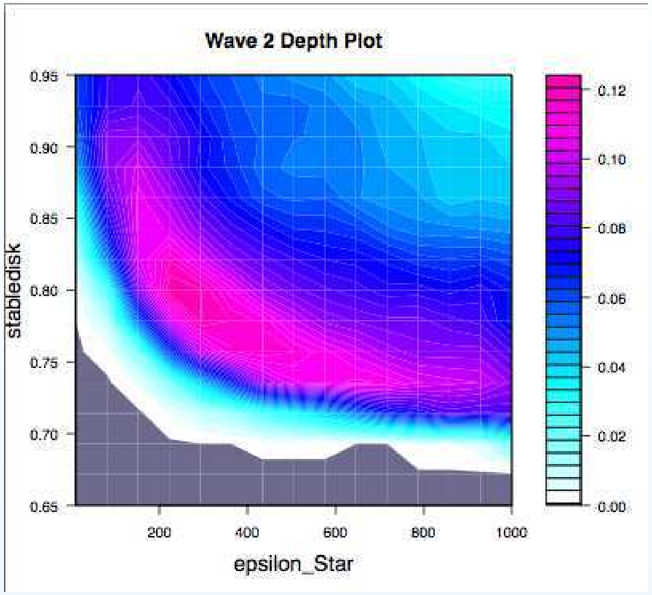

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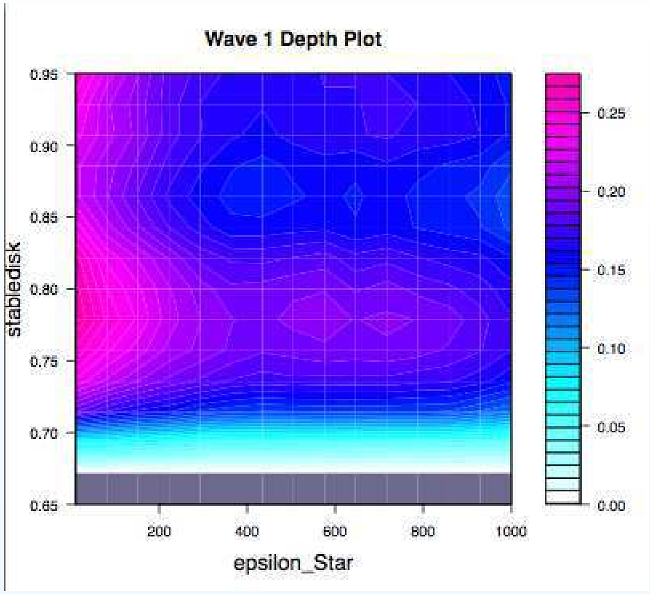

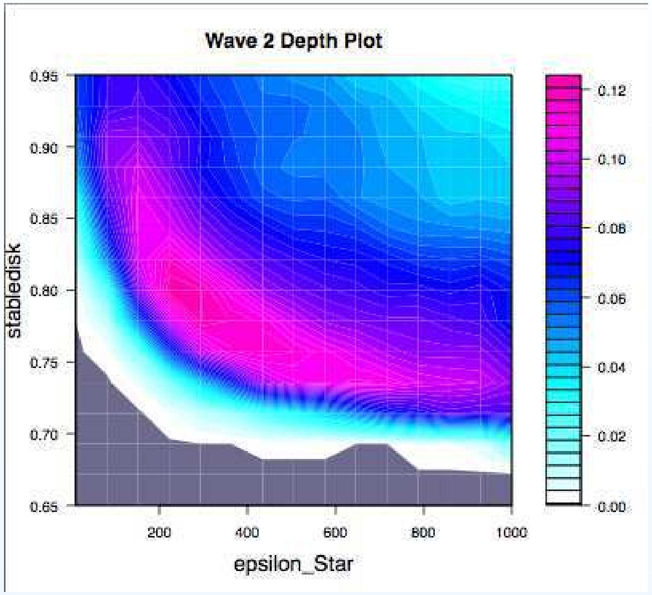

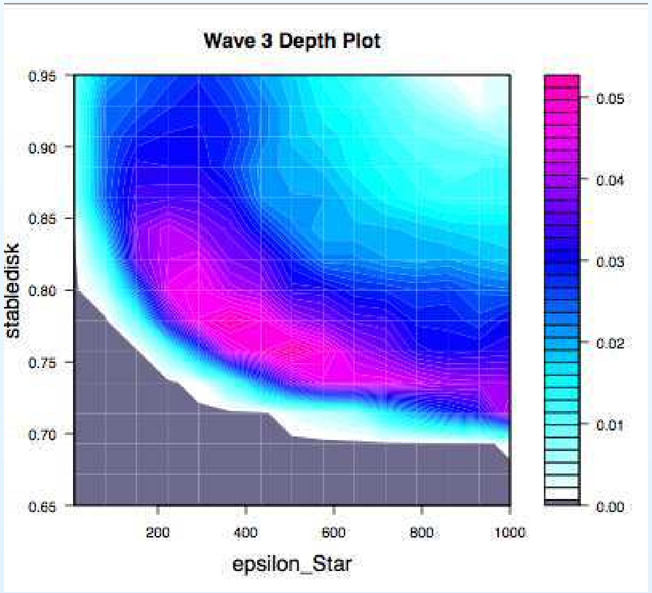

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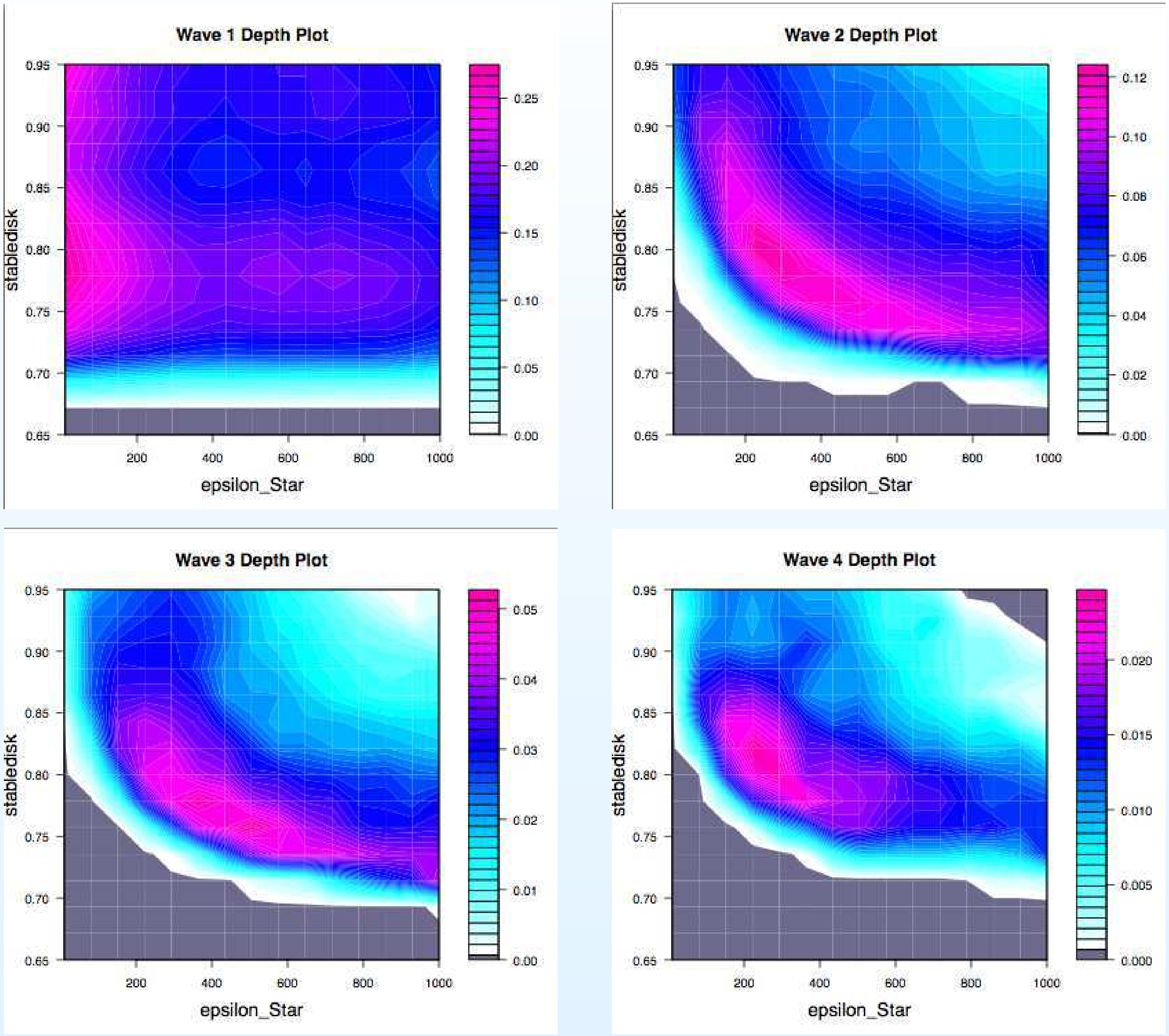

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[A] The difference between our simulator and the reified form.

[B] The difference between the reified form at the physically appropriate choice of x and the actual system behaviour y.

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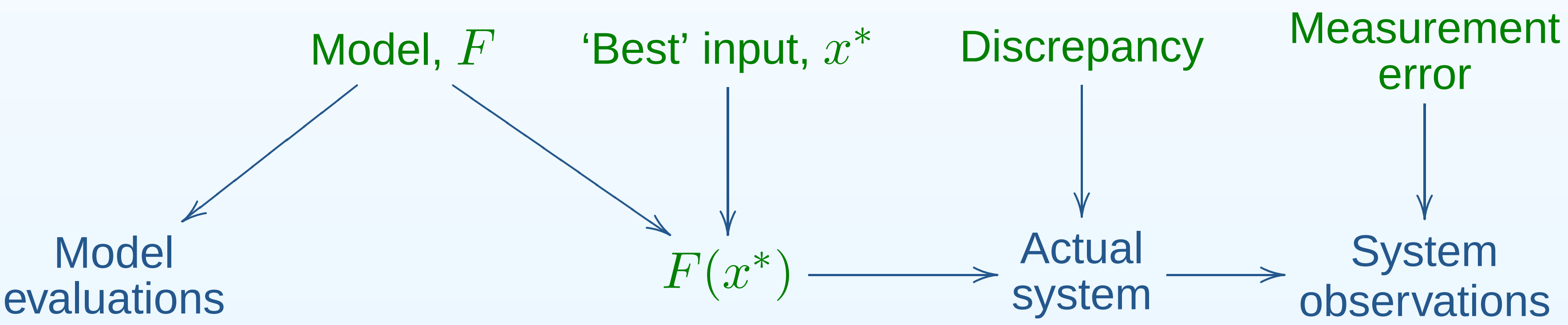

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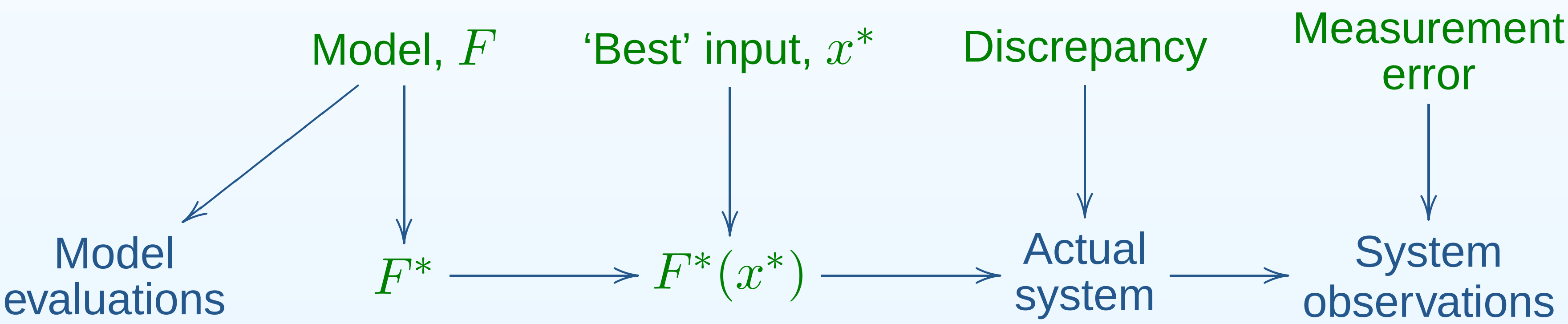

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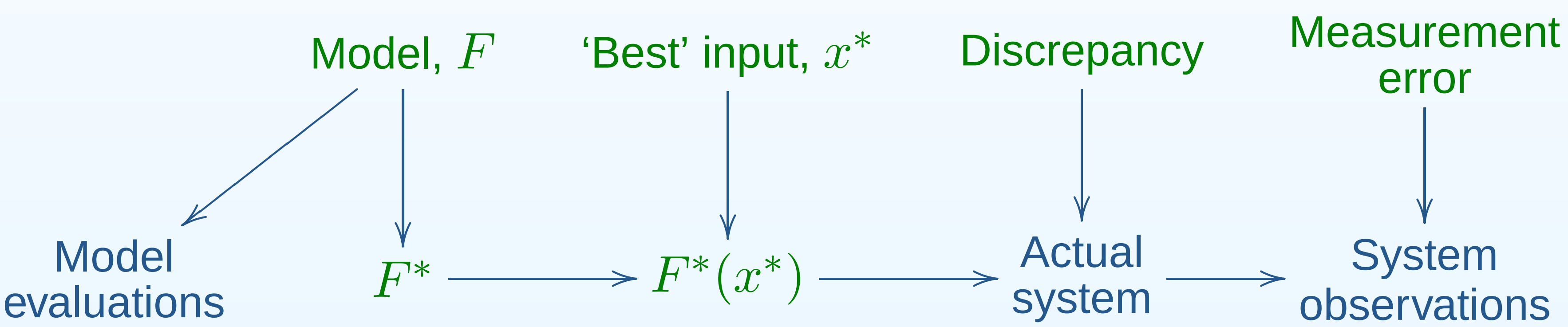

Reifying principle [2]

A collection of simulators $F_1, F_2, \ldots$ is jointly informative for y, as the simulators are jointly informative for F^*.

Linking F and F^* using emulators

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where we might model our judgements as $B^* = CB + \Gamma$, correlate $u(x)$ and $u^*(x)$, while $u^*(x, w)$, with additional parameters, w, is uncorrelated with remainder.

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Structured reification improves on this with systematic modelling for all aspects of model deficiency whose effects we can consider explicitly.

All our calibration and forecasting methodology is unchanged - all that has changed is our description of the joint covariance structure.

A Reified influence diagram

$$\left[F^{1}_{h:[n]}(x), \ldots, F^{m}_{h:[n]}(x)\right]$$

Evaluations of the simulator at each of m initial conditions
for historical components of simulator

A Reified influence diagram

$$\left[F^1_{h:[n]}(x), \ldots, F^m_{h:[n]}(x)\right] \longrightarrow F_{h:\text{suff}} \longrightarrow F^*_{h:\text{suff}} \longrightarrow f^*_h(x)$$

Global information $F_{\text{h:suff}}$ (from second order exchangeability modelling).
passes to Reified global form and to reified emulator.

A Reified influence diagram

$$\begin{tikzcd}
 & & & & & & e \arrow[d] \\
\left[F^1_{h:[n]}(x), \ldots, F^m_{h:[n]}(x)\right] \arrow[r] & F_{h:\mathrm{suff}} \arrow[r] & F^*_{h:\mathrm{suff}} \arrow[r] & f^*_h(x) \arrow[r] & F^*_h(x^*) \arrow[r] & y_h \arrow[r] & z \\
 & & & & & \epsilon_h \arrow[u] & \\
 & & & & x^* \arrow[uu] & &
\end{tikzcd}$$

Link with x^* to reified function, at true initial condition, linked to data z

A Reified influence diagram

$$\begin{tikzcd}
 & & & & \mathrm{MME} & & e \arrow[d] \\
\left[F^1_{h:[n]}(x), \ldots, F^m_{h:[n]}(x)\right] \arrow[r] & F_{h:\mathrm{suff}} \arrow[r] & F^*_{h:\mathrm{suff}} \arrow[r] & f^*_h(x) \arrow[r] & F^*_h(x^*) \arrow[u] \arrow[r] & y_h \arrow[r] & z \\
 & & & & x^* \arrow[u] & \epsilon_h \arrow[u] &
\end{tikzcd}$$

Add observation of a related multi-model ensemble (MME) consisting of tuned runs from related models (more exchangeability modelling).

A Reified influence diagram

$$
\begin{tikzcd}
 & & & & \mathrm{MME} & & e \arrow[d] \\
\left[F^1_{h:[n]}(x), \ldots, F^m_{h:[n]}(x)\right] \arrow[r] & F_{h:\mathrm{suff}} \arrow[r] & F^*_{h:\mathrm{suff}} \arrow[r] & f^*_h(x) \arrow[r] & F^*_h(x^*) \arrow[r] \arrow[u] & y_h \arrow[r] & z \\
 & & & & & \epsilon_h \arrow[u] & \\
 & & & & x^* \arrow[uu] & & \\
F'_{h:[n]}(x) \arrow[r] & F'_{h:\mathrm{suff}} \arrow[uuu] & & & & &
\end{tikzcd}
$$

Add a set of evaluations from a fast approximation

A Reified influence diagram

$$
\begin{tikzcd}
 & & & & \textcolor{red}{\mathrm{MME}} & & e \arrow[d] \\
\textcolor{red}{\left[F^1_{h:[n]}(x), \ldots, F^m_{h:[n]}(x)\right]} \arrow[r] & F_{h:\mathrm{suff}} \arrow[r] & F^*_{h:\mathrm{suff}} \arrow[r] & f^*_h(x) \arrow[r] & F^*_h(x^*) \arrow[u] \arrow[r] & y_h \arrow[r] & \textcolor{red}{z} \\
 & & & & & \epsilon_h \arrow[u] & \\
 & & & & x^* \arrow[uu] & & \\
\textcolor{red}{F'_{h:[n]}(x)} \arrow[r] & F'_{h:\mathrm{suff}} \arrow[uuu] & & & & & \\
\textcolor{red}{F'_{p:[n]}(x, d)} \arrow[r] & F'_{p:\mathrm{suff}} \arrow[u] & & & & &
\end{tikzcd}
$$

Add evaluations of fast simulator for outcomes to be predicted, with decision choices $\textcolor{red}{d}$

A Reified influence diagram

$$\begin{tikzcd}
 & & & & \mathrm{MME} & & e \arrow[d] \\
\left[F^1_{h:[n]}(x), \ldots, F^m_{h:[n]}(x)\right] \arrow[r] & F_{h:\mathrm{suff}} \arrow[r] & F^*_{h:\mathrm{suff}} \arrow[r] \arrow[dddd] & f^*_h(x) \arrow[r] & F^*_h(x^*) \arrow[r] \arrow[u] & y_h \arrow[r] & z \\
 & & & & & \epsilon_h \arrow[u] & \\
 & & & & x^* \arrow[uu] & & \\
F'_{h:[n]}(x) \arrow[r] & F'_{h:\mathrm{suff}} \arrow[uuu] & & & & & \\
F'_{p:[n]}(x, d) \arrow[r] & F'_{p:\mathrm{suff}} \arrow[r] \arrow[u] & F^*_{p:\mathrm{suff}} & & & &
\end{tikzcd}$$

Link to reified global terms for quantities to be predicted

A Reified influence diagram

$$
\begin{tikzcd}
& & & & \mathrm{MME} & & e \arrow[d] \\
\left[F^1_{h:[n]}(x), \ldots, F^m_{h:[n]}(x)\right] \arrow[r] & F_{h:\mathrm{suff}} \arrow[r] & F^*_{h:\mathrm{suff}} \arrow[r] \arrow[dddd] & f^*_h(x) \arrow[r] \arrow[dddd] & F^*_h(x^*) \arrow[r] \arrow[u] & y_h \arrow[r] & z \\
& & & & & \epsilon_h \arrow[u] & \\
& & & & x^* \arrow[uu] & & \\
F'_{h:[n]}(x) \arrow[r] & F'_{h:\mathrm{suff}} \arrow[uuu] & & & & & \\
F'_{p:[n]}(x, d) \arrow[r] & F'_{p:\mathrm{suff}} \arrow[r] \arrow[u] & F^*_{p:\mathrm{suff}} \arrow[r] & f^*_p(x, d) & & &
\end{tikzcd}
$$

And to reified global emulator, based on inputs and decisions

A Reified influence diagram

$$
\begin{tikzcd}
& & & & \color{red}{\mathrm{MME}} & & e \arrow[d] \\
\color{red}{\left[F^1_{h:[n]}(x), \ldots, F^m_{h:[n]}(x)\right]} \arrow[r] & F_{h:\mathrm{suff}} \arrow[r] & F^*_{h:\mathrm{suff}} \arrow[r] \arrow[dddd] & f^*_h(x) \arrow[r] \arrow[dddd] & F^*_h(x^*) \arrow[r] \arrow[u] & y_h \arrow[r] & \color{red}{z} \\
& & & & & \epsilon_h \arrow[u] \arrow[dd] & \\
& & & & x^* \arrow[uu] \arrow[dd] & & \\
\color{red}{F'_{h:[n]}(x)} \arrow[r] & F'_{h:\mathrm{suff}} \arrow[uuu] & & & & \epsilon_p \arrow[d] & \\
\color{red}{F'_{p:[n]}(x,d)} \arrow[r] & F'_{p:\mathrm{suff}} \arrow[u] \arrow[r] & F^*_{p:\mathrm{suff}} \arrow[r] & f^*_p(x,d) \arrow[r] & F^*_p(x^*,d^*) \arrow[r] & y_p \arrow[d] & \\
& & & & \boxed{d^*} \arrow[u] & \color{green}{C} &
\end{tikzcd}
$$

And link, through true future values y_p, to the overall utility cost C of making decision choice d^* [Attach more models to diagram at $F^*(x^*)$]

Concluding comments

To assess our uncertainty about complex systems, it is enormously helpful to have an overall (Bayesian) framework to unify all of the sources of uncertainty.

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Such analysis poses serious challenges, but they are no harder than all of the other modelling, computational and observational challenges involved with studying complex systems.

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Such analysis poses serious challenges, but they are no harder than all of the other modelling, computational and observational challenges involved with studying complex systems.

In particular,
Bayesian multivariate, multi-level, multi-model emulation,
careful structural discrepancy modelling
and iterative history matching
gives a great first pass treatment for most large modelling problems.

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